substance: NiO
property: phonon dispersion, phonon wavenumbers

phonon dispersion curves: Fig. 1, calculations: [75R, 76C, 79A], density of states: Fig. 2.

wavenumbers of infrared active phonons

$(\nu/c)_{TO}$	400 cm^{-1}	RT	green NiO		65G
	440 cm^{-1}		black NiO		
	387(5) cm^{-1}			neutron study, $(\nu/c)_{TO}(\Gamma)$	75R
$(\nu/c)_{LO}$	580 cm^{-1}		green NiO		65G
	560 cm^{-1}		black NiO		
	577(7) cm^{-1}			neutron study, $(\nu/c)_{LO}(\Gamma)$	75R

wavenumbers of Raman active phonons

$(\nu/c)_R$	400 cm^{-1}	black NiO		71D
	500 cm^{-1}			
	1100 cm^{-1}		assigned to 2 $(\nu/c)_{LO}$	
	1560 cm^{-1}		assigned to two-magnon peak with cut-off at 1880 cm^{-1}	

reststrahlen frequency

ν	$12.2 \cdot 10^{12}$ Hz	65G
	$11.45 \cdot 10^{12}$ Hz	75R

References:

65G Gielisse, P. J., Plendl, J. N., Mansur, L. C., Marshall, R., Mitra, S. S., Mykolojewicz, R., Smakula, A.: J. Appl. Phys. 36 (1965) 2446.

71D Dietz, R. E., Parisot, G. I., Meisner, A. E.: Phys. Rev. B4 (1971) 2302.

75R Reichardt, W., Wagner, V., Kress, W.: J. Phys. C8 (1975) 3955.

76C Coy, R. A., Thompson, C. W., Girman, E.: Solid State Commun. 18 (1976) 845.

79A Agarwal, S.: Solid State Commun. 29 (1979) 197.

Fig. 1.

NiO. Phonon dispersion curves, experimental data from neutron scattering, solid curves theoretical shell-model best fit [75R].

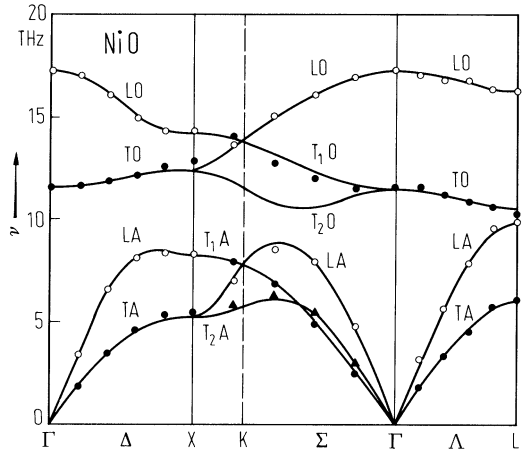

Fig. 2.

NiO. Phonon density of states vs. frequency [76C].